Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

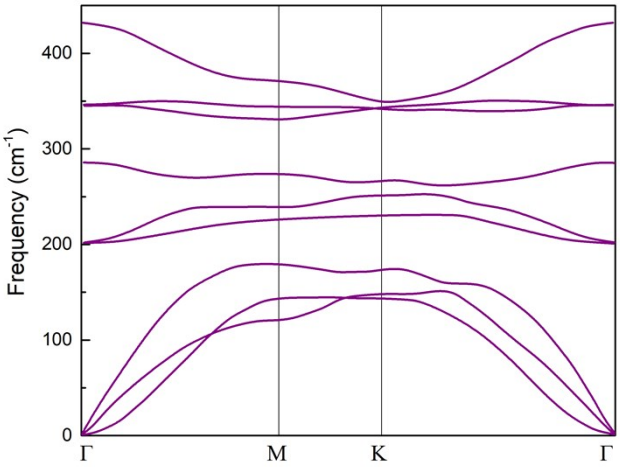

Fig. S1 Phonon band structure of MoSSe monolayer.

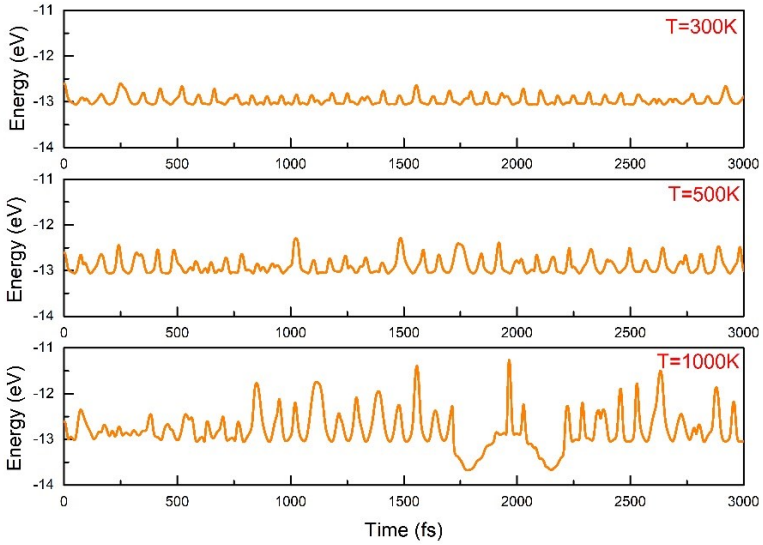

Fig. S2 The energy of MoSSe as a function of the AIMD time at 300 K, 500 K and 1000K.

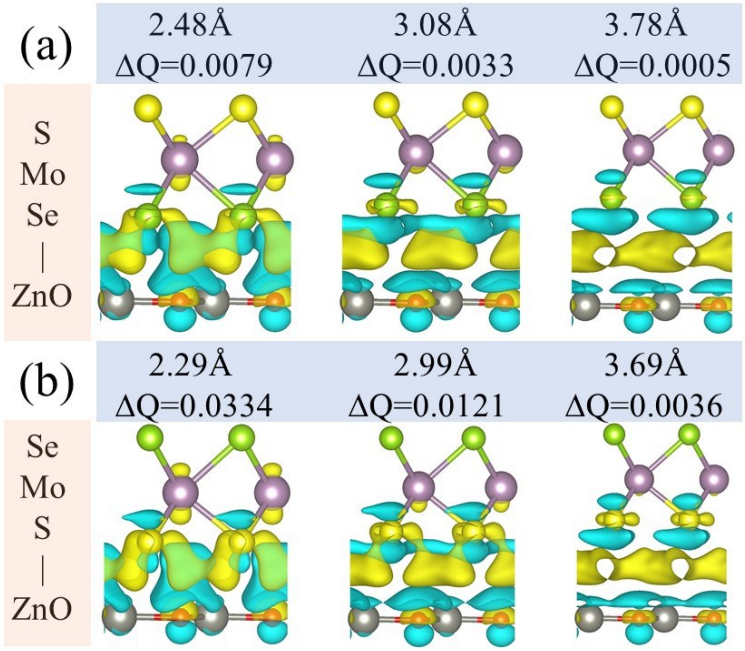

Fig. S3. The three-dimensional (3D) isosurface CDD and charge transfer ΔQ of (a) ZnO-SeMoS and (b) ZnO-SMoSe vdWHs under different interlayer distance. The isosurface values are 5.20×10^{-4} (6.21×10^{-4}), 1.96×10^{-4} (1.90×10^{-4}) and 6.27×10^{-5} (5.8×10^{-5}) eÅ^{-3} for ZnO-SeMoS (ZnO-SMoSe) at the interlayer distance of 2.48(2.29), 3.08(2.99) and 3.78(3.69) Å, respectively.

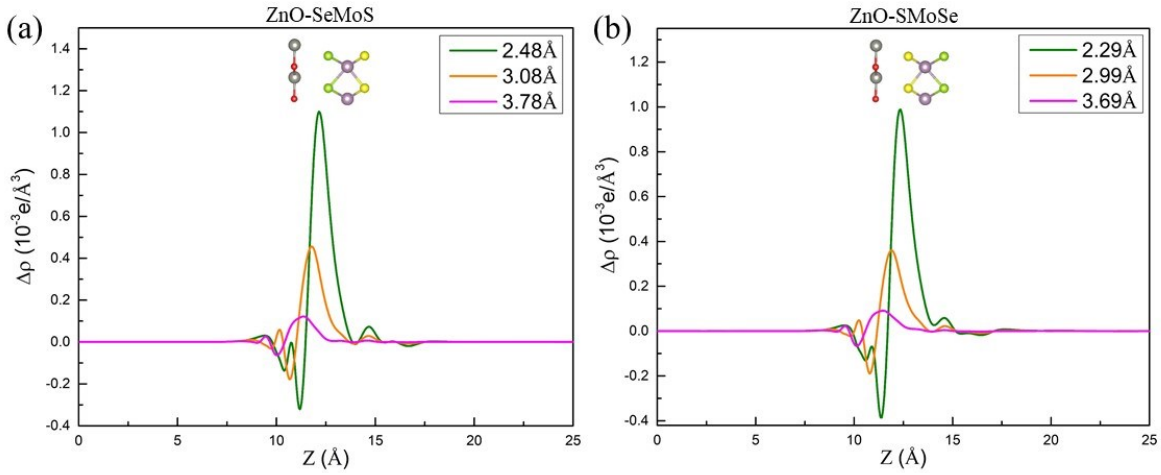

Fig. S4. The plane-averaged CDD of (a) ZnO-SeMoS and (b) ZnO-SMoSe vdWHs under different interlayer distance.